Negative differential thermal resistance and thermal transistor

Baowen Li

Department of Physics and Center for Computational Science and Engineering,
National University of Singapore, Singapore 117542, Republic of Singapore
Laboratory of Modern Acoustics and Institute of Acoustics, Nanjing University, 210093, PR China
NUS Graduate School for Integrative Sciences and Engineering, Singapore 117597, Republic of Singapore

Lei Wang

Department of Physics and Center for Computational Science and Engineering,
National University of Singapore, Singapore 117542, Republic of Singapore

Giulio Casati

Department of Physics and Center for Computational Science and Engineering,
National University of Singapore, Singapore 117542, Republic of Singapore
International Center for Nonlinear and Complex Systems,
Universita' degli studi dell'Insubria, Como, Italy,
Istituto Nazionale di Fisica della Materia, Unita' di Como,
and Istituto Nazionale di Fisica Nucleare, sezione di Milano, Milano, Italy
(Dated: 12 December 2005, revised 3 March 2006, to appear in Appl. Phys. Lett.)

We report on the first model of a thermal transistor to control heat flow. Like its electronic counterpart, our thermal transistor is a three-terminal device with the important feature that the current through the two terminals can be controlled by small changes in the temperature or in the current through the third terminal. This control feature allows us to switch the device between "off" (insulating) and "on" (conducting) states or to amplify a small current. The thermal transistor model is possible because of the negative differential thermal resistance.

The invention of the transistor[1] and other relevant devices that control the electric charge flow has led to an impressive technological development. In recent years some interesting progress has been made also in the control of the heat current. Indeed a theoretical model of a thermal rectifier has been recently proposed[2] in which the heat can flow preferentially in one direction. More recently, new models of thermal diode have been devised[3, 4] which allows to improve the efficiency by more than three orders of magnitude.

In this Letter we propose a model for a thermal transistor which can control the heat flow in analogy to the usual electric transistor for the control of the electric current. The reason why such a device can, in principle, operate is grounded in the phenomenon of "*negative differential thermal resistance*" (NDTR)which, as shown below, can take place in nonlinear lattices.

Our model of thermal transistor consists of three segments, D, S and G. (see Figure 1(a) for its configuration). The names D, S and G follow from the ones used in a MOSFET (Metal-Oxide-Semiconductor Field-Effect-Transistor). Each segment is a Frenkel-Kontorova (FK) lattice [5, 6]. Segments S and D are coupled (usually weakly) via a spring of constant k_{int}, while Segment G, the control segment, is coupled to the junction particle O between segments S and D via a spring of constant k_{int_G}. Temperature T_G is used to control temperature T_O (at the junction O) which determines the heat current from

D to S. The total Hamiltonian of the model writes:

$$
\begin{aligned}
H &= H_S + H_D + H_G + H_{int} + H_{int_G} \\
&= \sum_{i=1}^{N_S} \frac{1}{2}\dot{x}_{S,i}^2 + \frac{1}{2}k_S(x_{S,i} - x_{S,i-1})^2 - \frac{V_S}{(2\pi)^2}\cos 2\pi x_{S,i} \\
&+ \sum_{i=1}^{N_D} \frac{1}{2}\dot{x}_{D,i}^2 + \frac{1}{2}k_D(x_{D,i} - x_{D,i-1})^2 - \frac{V_D}{(2\pi)^2}\cos 2\pi x_{D,i} \\
&+ \sum_{i=1}^{N_G} \frac{1}{2}\dot{x}_{G,i}^2 + \frac{1}{2}k_G(x_{G,i} - x_{G,i-1})^2 - \frac{V_G}{(2\pi)^2}\cos 2\pi x_{G,i} \\
&+ \frac{1}{2}k_{int}(x_{S,N_S} - x_{D,N_D})^2 \\
&+ \frac{1}{2}k_{int_G}(x_{S,N_S} - x_{G,N_G})^2
\end{aligned}
\tag{1}
$$

Here $x_{D,i}$, $x_{S,i}$, and $x_{G,i}$ are the particles' displacements from their equilibrium positions in segment D, S and G, respectively. Fixed boundaries conditions are taken, i.e., $x_{D,0} = x_{S,0} = x_{G,0} = 0$.

In the following we will present first the results of our numerical simulations, then the theoretical explanation. In our numerical simulations the lattices are coupled, at their first particles, with heat baths at different temperatures T_D, T_S and T_G, respectively. We use Langevin heat baths and we have checked that our results do not depend on the particular heat bath realization (e.g. Nose-Hoover heat baths). The local heat flux is defined by
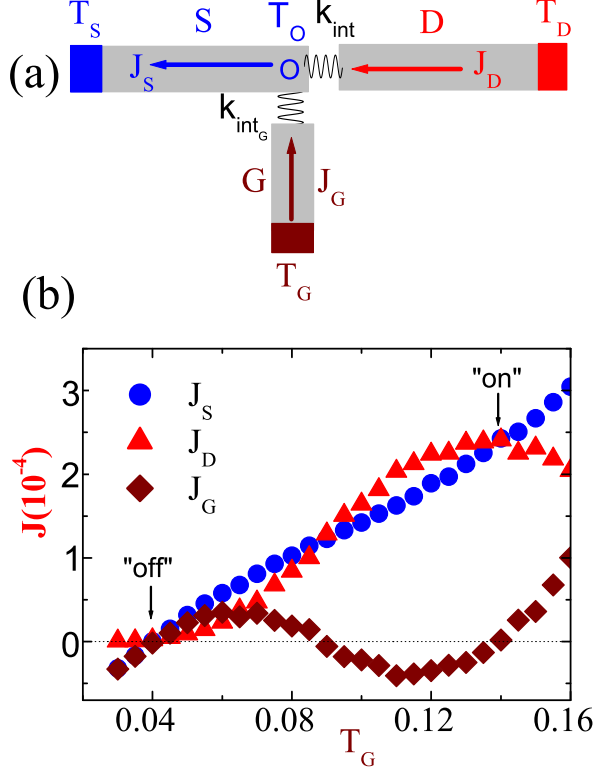
FIG. 1: (a) Configuration of the thermal transistor. (b) Heat current versus the control temperature T_G. Parameters are: T_D=0.2, V_D=1.0, k_D=0.2, k_{int}=0.05; T_S=0.04, V_S=5, k_S=0.2, V_G=5, k_G=1, k_{int_G}=1. Notice that in a wide region both J_S and J_D increase when the temperature T_G is increased.

$J_n \equiv k \langle \dot{x}_n (x_n - x_{n-1}) \rangle$ and the local temperature is defined as $T_n = \langle \dot{x}_n^2 \rangle$. The simulations are performed long enough to allow the system to reach a non-equilibrium steady state where the local heat flux is constant in each segment.

As illustrated in Figures 1-2, the model described by Hamiltonian (1) can exhibit different useful functions depending on the parameters values.

Thermal Switch: We first demonstrate the "*switch*" function of our transistor, namely we show that the system can act like a good heat conductor or an insulator depending on the control temperature T_G. This is shown in Figure 1(b), where we plot J_G, J_S, and J_D versus T_G. When T_G increases from 0.03 to 0.135, both J_D and J_S increase. In particular, at three points: $T_G \approx$ 0.04, 0.09 and 0.135, we have that $J_D = J_S$ and thus J_G is exactly zero. These three points correspond to "off", "semi-on" and "on" states, at which J_D is 2.4×10^{-6}, 1.2×10^{-4} and 2.3×10^{-4}, respectively. The ratio of the heat currents at the "on" and "off" states is about 100, hence our model displays one important function - switch - just like the function of a MOSFET used in a digital circuit.
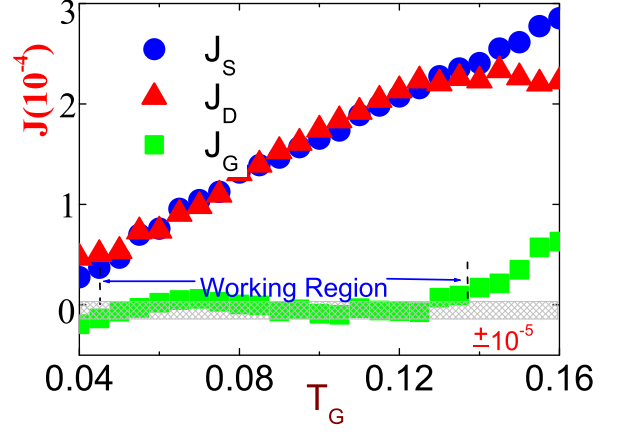
Thermal modulator/amplifier: As demonstrated

FIG. 2: Heat current versus the control temperature T_G. Here: T_D=0.2, V_D=1.0, k_D=0.2, T_S=0.04, V_S=5, k_S=0.2, k_{int}=0.05, V_G=5, k_G=1, k_{int_G}=0.1. The shadow region is the range of variation of J_G in the temperature interval $T_G \in (0.05, 0.135)$.

above, the heat current from D to S can be switched between different values. However, in many cases, like in an analog circuit, one needs to continuously adjust the current in a wide range. In Figure 2 we demonstrate this "modulator/amplifier" function of our transistor. Here it is seen that in the temperature interval $T_G \in (0.05, 0.135)$, the heat current through the segment G remains very small ($-10^{-5} \sim 10^{-5}$), within the shadow strip in Figure 2, while the heat currents J_S and J_D are continuously controlled from 5×10^{-5} to 2×10^{-4}.

Let us now turn to the discussion of the underlying physical mechanism which allows the transistors function. In all cases considered here, the heat resistance of segment G has been taken small enough so that $T_O \approx T_G$. For fixed thermal baths temperatures T_S and T_D, we would like now to understand how the heat currents J_S and J_D depend on temperature T_O. This dependence is determined by the differential thermal resistance, $R_S = \left(\frac{\partial J_S}{\partial T_O} \right)^{-1}_{T_S = \text{const}}$ and $R_D = - \left(\frac{\partial J_D}{\partial T_O} \right)^{-1}_{T_D = \text{const}}$. In typical situations the heat current increases with the increase of the thermal gradient and therefore both R_S and R_D are positive. As a consequence, the "*current amplification factor*",

$$\alpha \equiv \left| \frac{\partial J_D}{\partial J_G} \right| = \left| \frac{R_S}{R_S + R_D} \right| < 1, \qquad (2)$$

namely, in order to induce a change ΔJ_D, the control heat bath has to provide a larger ΔJ_G. This means that the "transistor" can never work!

In order to get the amplification effect, namely $\alpha > 1$, either R_S or R_D must be negative. Thus we must have a "*negative differential thermal resistance*" (NDTR). In such case the possibility arises that when T_O changes both J_S and J_D change simultaneously in the same way.
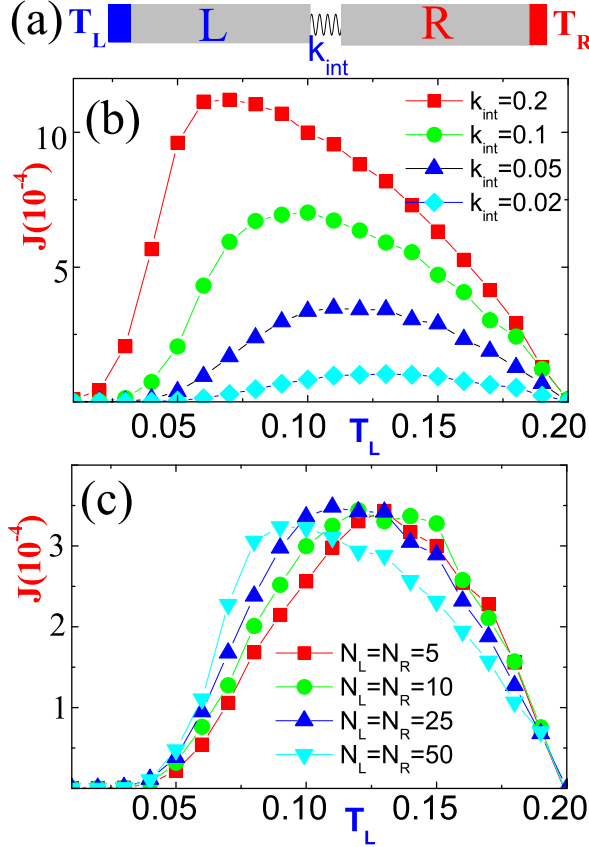
FIG. 3: (a) Configuration of the model exhibiting the negative differential thermal resistance (see definition in the text). (b) Heat current versus temperature T_L (at fixed $T_R=0.2$) for different coupling constants, k_{int}, with lattice size $N_L=N_R=25$. The system parameters are: $V_L=5$, $V_R=1$, $k_L=1$, $k_R=0.2$. (c) Same as (b) but for different system sizes and $k_{int}=0.05$. Notice that when $T_L \leq 0.1$ the heat current increases with decreasing the external temperature difference.

Therefore the condition $J_S=J_D$ can be achieved for several different values of T_O (as shown in Figure 1). Analogously, the condition $J_S \approx J_D$ can be verified in a wide range of T_O (as shown in Figure 2). In these situations heat switch and heat modulator/amplifier are possible. In the ideal, limiting case of $R_S=-R_D$ which, in principle, can be obtained by adjusting parameters, the transistor works perfectly.

Figure 3 illustrates the mechanism of NDTR. In Figure 3(b) we plot the heat current versus temperature T_L (see Figure 3(a))for fixed T_R, fixed lattice size and for different coupling constants k_{int} . In Figure 3(c) instead the heat current is plotted for different lattice sizes with fixed coupling constants k_{int}.

As it is clearly seen, in a wide range of system parameters, for a fixed temperature T_R, there exists a temperature interval in which a larger value of $T_L(< T_R)$, corresponding to a smaller thermal gradient, can induce a larger heat current.

The phenomenon of NDTR can be understood from the mismatch between the phonon bands of the two interface particles. This is illustrated in Figure 4 where we plot the power spectra of the two interface particles at different temperatures T_L for a fixed $T_R=0.2$ (Figure 3(a)). As it is seen, the overlap of the power spectra increases as T_L increases i.e. as the thermal gradient decreases. Therefore, by increasing T_L we are in the presence of two competing effects: from one hand the thermal gradient decreases; on the other hand the band overlap increases. The beaviour of the heat current depends on which of these two effects prevails. In particular the phenomenon of NDTR can take place.

The physical mechanism of such behaviour is due to the fact that the variation of the bands position with temperature depends on the strength of nonlinearity. This general property is at the base of the thermal diode models [3, 4]. In particular, for the model discussed in this paper, as the temperature T_L increases, the kinetic energy of the left interface particle becomes large enough to overcome the on site potential barrier and low frequency modes appear.

Finally, we would like to discuss the possibility of building a thermal transistor in real physical systems and the possible applications. Due to the fast developing semiconductor technology, it is now possible to fabricate several low dimensional devices, such as nanotubes, nanowires and thin films in nanometer scale[7]. A nanotube with small diameter or a nanowire is basically a one dimensional heat conductor. For the purpose of our model, which is indeed one dimensional, one can fabricate a T-shape nanotube or nanowire. To build the on-side potential in the FK model, one may put different segments of nanotubes/nanowires on the surface of different substrates.

Among the possible applications we would like to mention, as an example, that in our model, by adjusting the temperature of the third terminal, one can amplify the current through the other two terminals. This can be used as an efficient heat pump to dissipate heat from a microelectronic or nanoelectronic device where a large amount of redundant heat is produced due to the fast operational speed of the device. This could be very important since, as it is known, the redundant heat, if it is not dissipated immediately, may deteriorate the device.

In conclusion, we have built a theoretical model for a thermal transistor. The model displays two basic functions of a transistor: switch and modulator/amplifier. The crucial element of the thermal transistor is the *negative differential thermal resistance*. Although at present this is no more than an abstract model, we believe that, sooner or later, it can be realized in a nanoscale system experiment. After all the Frenkel-Kontorova model used in our simulations is a very popular model in condensed matter physics[5, 6]. For instance, it has been used to
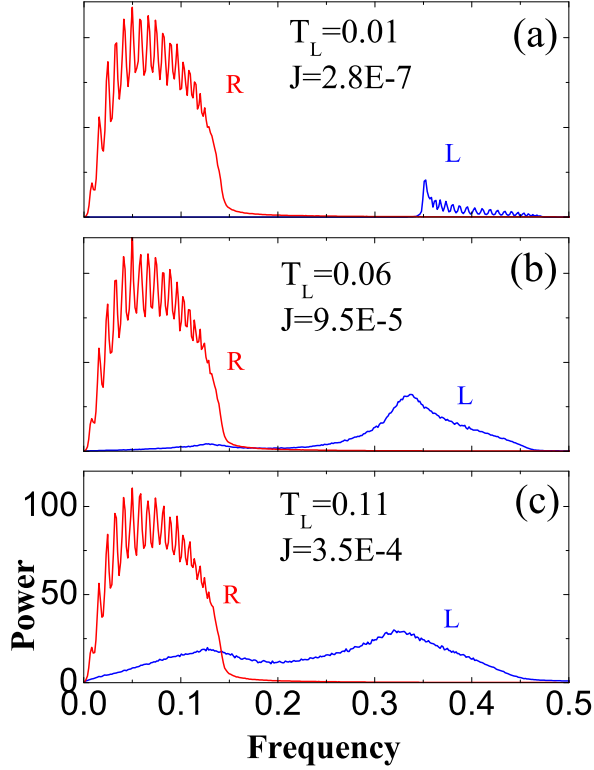
FIG. 4: The power spectra of the particles at the right (R) side and the left (L) side of the interface, for different temperature T_L with fixed T_R=0.2. The system parameters are: V_L=5, V_R=1, k_L=1, k_R=0.2, k_{int}=0.05, N=50. Notice that the overlap of the spectra increases as the temperature T_L increases, which results in the increase of the heat current with decreasing the external temperature difference when $T_L \leq 0.11$.

model crystal dislocations, epitaxial monolayers on the crystal surface, ionic conductors and glassy materials, an electron in a quasi-1D metal below the Peierls transition, charge density waves, Josephson junctions chains, and dry friction. More recently, this model has been employed to study transport properties of vortices in easy flow channels[8] and strain-mediated interaction of vacancy lines in a pseudomorphic adsorbate system[9].

[1] J. Bardeen and W. H. Brattain, Phys. Rev. **74**, 230 (1948).

[2] M. Terraneo, M. Peyrard, and G. Casati, Phys. Rev. Lett **88**, 094302 (2002).

[3] B. Li, L. Wang, and G. Casati, Phys. Rev. Lett. **93**, 184301 (2004).

[4] B. Li, J.-H Lan,, and L. Wang, Phys. Rev. Lett. **95**, 104302 (2005).

[5] V. L. Pokrovsky and A. L. Talapov, Theory of Incommensurate Crystals, Soviet Scientific Reviews Supplement Series, Physics Vol. 1 (Harwood, New York, 1984).

[6] O. M. Braun and Y. S. Kivshar, Phys. Rep. **306**, 1 (1998).

[7] D. G. Cahill *et al.* J. Appl. Phys, **93**, 793 (2003).

[8] R. Besseling, R. Niggebrugge, and P. H. Kes, Phys. Rev. Lett. **82**, 3144 (1999).

[9] S. C. Erwin, A. A. Baski, L. J. Whitman, and R. E. Rudd, Phys. Rev. Lett. **83**, 1818 (1999).